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\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	Jun 03	New e-mail delivery for search results now available
NEWS	4	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS	5	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
NEWS	6	Aug 26	Sequence searching in REGISTRY enhanced
NEWS	7	Sep 03	JAPIO has been reloaded and enhanced
NEWS	8	Sep 16	Experimental properties added to the REGISTRY file
NEWS	9	Sep 16	CA Section Thesaurus available in CAPLUS and CA
NEWS	10	Oct 01	CASREACT Enriched with Reactions from 1907 to 1985
NEWS	11	Oct 24	BEILSTEIN adds new search fields
NEWS	12	Oct 24	Nutraceuticals International (NUTRACEUT) now available on STN
NEWS	13	Nov 18	DKILIT has been renamed APOLLIT
NEWS	14	Nov 25	More calculated properties added to REGISTRY
NEWS	15	Dec 04	CSA files on STN
NEWS	16	Dec 17	PCTFULL now covers WP/PCT Applications from 1978 to date
NEWS	17	Dec 17	TOXCENTER enhanced with additional content
NEWS	18	Dec 17	Adis Clinical Trials Insight now available on STN
NEWS	19	Jan 29	Simultaneous left and right truncation added to COMPENDEX, ENERGY, INSPEC
NEWS	20	Feb 13	CANCERLIT is no longer being updated
NEWS	21	Feb 24	METADEx enhancements
NEWS	22	Feb 24	PCTGEN now available on STN
NEWS	23	Feb 24	TEMA now available on STN
NEWS	24	Feb 26	NTIS now allows simultaneous left and right truncation
NEWS	25	Feb 26	PCTFULL now contains images
NEWS	26	Mar 04	SDI PACKAGE for monthly delivery of multifile SDI results
NEWS	27	Mar 20	EVENTLINE will be removed from STN
NEWS	28	Mar 24	PATDPAFULL now available on STN
NEWS	29	Mar 24	Additional information for trade-named substances without structures available in REGISTRY
NEWS	30	Apr 11	Display formats in DGENE enhanced
NEWS	31	Apr 14	MEDLINE Reload
NEWS	32	Apr 17	Polymer searching in REGISTRY enhanced
NEWS	33	Jun 13	Indexing from 1947 to 1956 added to records in CA/CAPLUS
NEWS	34	Apr 21	New current-awareness alert (SDI) frequency in WPIDS/WPINDEX/WPIX
NEWS	35	Apr 28	RDISCLOSURE now available on STN
NEWS	36	May 05	Pharmacokinetic information and systematic chemical names added to PHAR
NEWS	37	May 15	MEDLINE file segment of TOXCENTER reloaded
NEWS	38	May 15	Supporter information for ENCOMPAT and ENCOMPLIT updated
NEWS	39	May 16	CHEMREACT will be removed from STN
NEWS	40	May 19	Simultaneous left and right truncation added to WSCA
NEWS	41	May 19	RAPRA enhanced with new search field, simultaneous left and

right truncation  
NEWS 42 Jun 06 Simultaneous left and right truncation added to CBNB  
NEWS 43 Jun 06 PASCAL enhanced with additional data  
NEWS 44 Jun 20 2003 edition of the FSTA Thesaurus is now available  
NEWS 45 Jun 25 HSDB has been reloaded

NEWS EXPRESS April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT  
MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),  
AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS INTER General Internet Information  
NEWS LOGIN Welcome Banner and News Items  
NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 14:54:19 ON 01 JUL 2003

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 14:54:29 ON 01 JUL 2003

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 30 JUN 2003 HIGHEST RN 540462-79-1

DICTIONARY FILE UPDATES: 30 JUN 2003 HIGHEST RN 540462-79-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> s irinotecan

L1 4 IRINOTECAN

=> d l1 fide

L1 ANSWER 1 OF 4 REGISTRY COPYRIGHT 2003 ACS

RN 209370-55-8 REGISTRY  
CN DNA (rabbit carboxyl esterase Irinotecan-activating cDNA plus flanks)  
(9CI) (CA INDEX NAME)

OTHER NAMES:

CN GenBank AF036930  
FS NUCLEIC ACID SEQUENCE  
MF Unspecified  
CI MAN  
SR GenBank  
LC STN Files: CA, CAPLUS, GENBANK

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*  
\*\*\* USE 'SQD' OR 'SQIDE' FORMATS TO DISPLAY SEQUENCE \*\*\*  
1 REFERENCES IN FILE CA (1957 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

=> d 11 2-4 fide

L1 ANSWER 2 OF 4 REGISTRY COPYRIGHT 2003 ACS  
RN 203173-72-2 REGISTRY  
CN [1,4'-Bipiperidine]-1'-carboxylic acid, (4S)-4-ethyl-3,4,12,14-tetrahydro-4-hydroxy-3,14-dioxo-11-(trimethylsilyl)-1H-pyrano[3',4':6,7]indolizino[1,2-b]quinolin-9-yl ester (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN [1,4'-Bipiperidine]-1'-carboxylic acid, 4-ethyl-3,4,12,14-tetrahydro-4-hydroxy-3,14-dioxo-11-(trimethylsilyl)-1H-pyrano[3',4':6,7]indolizino[1,2-b]quinolin-9-yl ester, (S)-

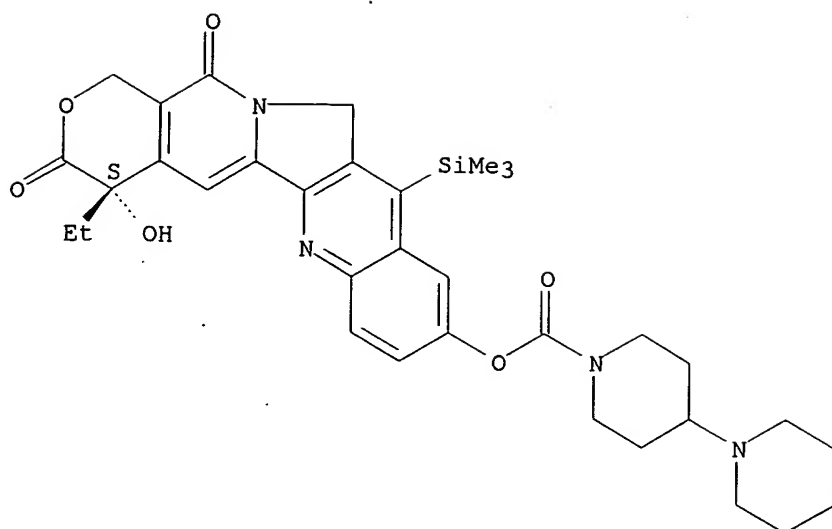
OTHER NAMES:

CN (20S)-7-(Trimethylsilyl)irinotecan  
FS STEREOSEARCH  
MF C34 H42 N4 O6 Si  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C5N	NC5	6	C5N	46.156.1	2
C4N-C5N-C5N-	NC4-NC5-NC5-	5-6-6-6-6	C18N2O	7726.21.4	1
C5O-C6	OC5-C6				

Absolute stereochemistry. Rotation (+).



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1	pH 1	(1) ACD
Bioconc. Factor (BCF)	4.72	pH 4	(1) ACD
Bioconc. Factor (BCF)	35.2	pH 7	(1) ACD
Bioconc. Factor (BCF)	293	pH 8	(1) ACD
Bioconc. Factor (BCF)	4855	pH 10	(1) ACD
Boiling Point (BP)	850.7+/-65.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	129.54+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	468.3+/-61.7 deg C		(1) ACD
H acceptors (HAC)	10		(1) ACD
H donors (HD)	1		(1) ACD
Koc (KOC)	1	pH 1	(1) ACD
Koc (KOC)	13.5	pH 4	(1) ACD
Koc (KOC)	101	pH 7	(1) ACD
Koc (KOC)	842	pH 8	(1) ACD
Koc (KOC)	13933	pH 10	(1) ACD
logD (LOGD)	0.57	pH 1	(1) ACD
logD (LOGD)	2.18	pH 4	(1) ACD
logD (LOGD)	3.05	pH 7	(1) ACD
logD (LOGD)	3.97	pH 8	(1) ACD
logD (LOGD)	5.19	pH 10	(1) ACD
logP (LOGP)	5.320+/-1.205		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	630.81		(1) ACD
pKa (PKA)	11.00+/-0.20	Most Acidic	(1) ACD
pKa (PKA)	9.33+/-0.20	Most Basic	(1) ACD
Vapor Pressure (VP)	18.75E-31 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

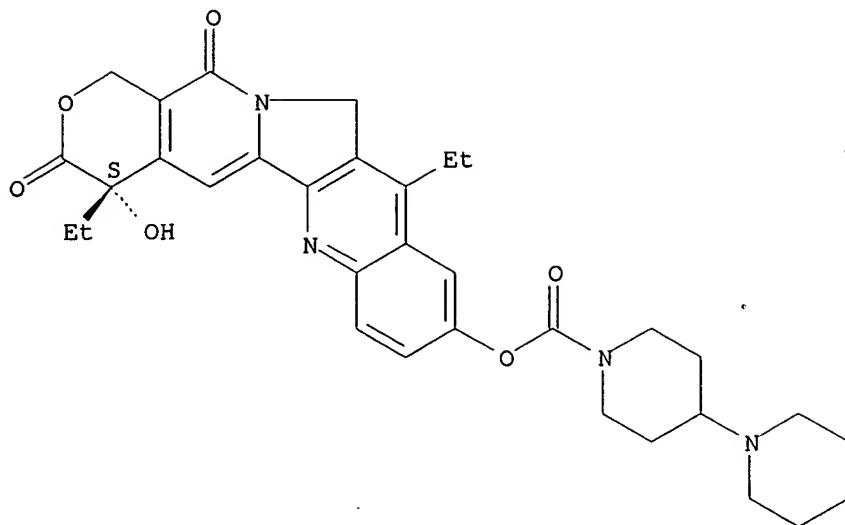
5 REFERENCES IN FILE CA (1957 TO DATE)  
5 REFERENCES IN FILE CAPLUS (1957 TO DATE)

L1 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2003 ACS  
RN 100286-90-6 REGISTRY  
CN [1,4'-Bipiperidine]-1'-carboxylic acid, (4S)-4,11-diethyl-3,4,12,14-tetrahydro-4-hydroxy-3,14-dioxo-1H-pyrano[3',4':6,7]indolizino[1,2-b]quinolin-9-yl ester, monohydrochloride (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN 1H-Pyrano[3',4':6,7]indolizino[1,2-b]quinoline, [1,4'-bipiperidine]-1'-carboxylic acid deriv.  
CN [1,4'-Bipiperidine]-1'-carboxylic acid, 4,11-diethyl-3,4,12,14-tetrahydro-4-hydroxy-3,14-dioxo-1H-pyrano[3',4':6,7]indolizino[1,2-b]quinolin-9-yl ester, monohydrochloride, (S)-  
OTHER NAMES:  
CN 7-Ethyl-10-[[4-(1-piperidyl)-1-piperidyl]carbonyloxy]camptothecin hydrochloride  
CN . Campto  
CN Camptothecin 11  
CN Camptothecin 11 hydrochloride  
CN CPT 11  
CN Irinotecan hydrochloride  
CN Topotecin  
CN U 101440E  
FS STEREOSEARCH  
DR 111348-33-5  
MF C33 H38 N4 O6 . Cl H  
SR CA  
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN\*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAPLUS, CBNB, CHEMCATS, CIN, CSCHEM, DDFU, DIOGENES, DRUGPAT, DRUGU, DRUGUPDATES, EMBASE, IPA, MEDLINE, MRCK\*, PHAR, PHARMASEARCH, PROMT, RTECS\*, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL  
(\*File contains numerically searchable property data)  
CRN (97682-44-5)

#### Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C5N	NC5	6	C5N	46.156.1	2
C4N-C5N-C5N	NC4-NC5-NC5	5-6-6-6-6	C18N2O	7726.21.4	1
C5O-C6	OC5-C6				

Absolute stereochemistry. Rotation (+).



● HCl

494 REFERENCES IN FILE CA (1957 TO DATE)

6 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

495 REFERENCES IN FILE CAPLUS (1957 TO DATE)

L1 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2003 ACS

RN 97682-44-5 REGISTRY

CN [1,4'-Bipiperidine]-1'-carboxylic acid, (4S)-4,11-diethyl-3,4,12,14-tetrahydro-4-hydroxy-3,14-dioxo-1H-pyrano[3',4':6,7]indolizino[1,2-b]quinolin-9-yl ester (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1H-Pyrano[3',4':6,7]indolizino[1,2-b]quinoline, [1,4'-bipiperidine]-1'-carboxylic acid deriv.

CN [1,4'-Bipiperidine]-1'-carboxylic acid, 4,11-diethyl-3,4,12,14-tetrahydro-4-hydroxy-3,14-dioxo-1H-pyrano[3',4':6,7]indolizino[1,2-b]quinolin-9-yl ester, (S)-

OTHER NAMES:

CN (+)-Irinotecan

CN Camptosar

CN Irinotecan

FS STEREOSEARCH

MF C33 H38 N4 O6

CI COM

SR CA

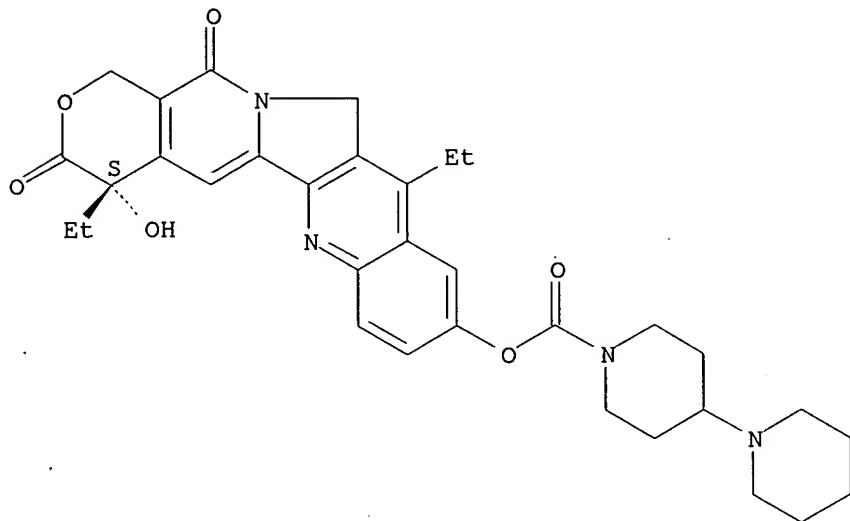
LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN\*, BIOBUSINESS, BIOSIS, CA, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CIN, CSCHEM, DDFU, DIOGENES, DRUGNL, DRUGPAT, DRUGU, DRUGUPDATES, IPA, MRCK\*, PROMT, RTECS\*, SYNTHLINE, TOXCENTER, USAN, USPAT2, USPATFULL  
 (\*File contains numerically searchable property data)

## Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count

C5N	NC5	6	C5N	46.156.1	2
C4N-C5N-C5N-	NC4-NC5-NC5-	5-6-6-6-6	C18N2O	7726.21.4	1
C5O-C6	OC5-C6				

Absolute stereochemistry. Rotation (+).



#### Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1	pH 1	(1) ACD
Bioconc. Factor (BCF)	1	pH 4	(1) ACD
Bioconc. Factor (BCF)	2.51	pH 7	(1) ACD
Bioconc. Factor (BCF)	20.9	pH 8	(1) ACD
Bioconc. Factor (BCF)	346	pH 10	(1) ACD
Boiling Point (BP)	873.4+/-65.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	132.98+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	482.0+/-61.7 deg C		(1) ACD
H acceptors (HAC)	10		(1) ACD
H donors (HD)	1		(1) ACD
Koc (KOC)	1	pH 1	(1) ACD
Koc (KOC)	1.61	pH 4	(1) ACD
Koc (KOC)	15.2	pH 7	(1) ACD
Koc (KOC)	127	pH 8	(1) ACD
Koc (KOC)	2102	pH 10	(1) ACD
logD (LOGD)	-1.11	pH 1	(1) ACD
logD (LOGD)	0.57	pH 4	(1) ACD
logD (LOGD)	1.54	pH 7	(1) ACD
logD (LOGD)	2.46	pH 8	(1) ACD
logD (LOGD)	3.68	pH 10	(1) ACD
logP (LOGP)	3.809+/-0.628		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD

Molecular Weight (MW)	586.68		(1) ACD
pKa (PKA)	11.00+/-0.20	Most Acidic	(1) ACD
pKa (PKA)	9.33+/-0.20	Most Basic	(1) ACD
Vapor Pressure (VP)	1.31E-32 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris  
V4.67 ((C) 1994-2003 ACD)

659 REFERENCES IN FILE CA (1957 TO DATE)

17 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

662 REFERENCES IN FILE CAPLUS (1957 TO DATE)